Celebrating 20 Years of Computational Science with PETSc Tutorial and Conference

Monday, June 15 – Thursday, June 18, 2015
Argonne National Laboratory, Building 240
http://www.mcs.anl.gov/petsc/petsc-20.pdf
Conference Announcement (http://www.mcs.anl.gov/petsc-20-announcement)

Conference Dinners: The cost for conference dinners (to be held at the Argonne Guest House on Monday and Tuesday at 6:30 pm) is $30 each. There will also be a cash bar. We will sell tickets (cash only) at the tutorial, at the conference, and at the door. Please let us know if you **do not plan** to attend either of the conference dinners so we can order the correct amount of food.

Lunches: Lunches on Tuesday and Wednesday will be at the Argonne cafeteria; attendees can pay with cash or credit card.

Discussion room and wifi: A room for rest, relaxation, and discussion will be available in the Building 240 conference center during the entire time of the tutorial and conference. Wifi is available in the conference center: attach to the "Guest" network and start your browser to register; no password is necessary.

PETSc Tutorial Schedule

Monday, June 15, 2015

7:30 – 8:15	Bus from Argonne Guest to Building 240 Conference Center
8:00 – 8:30	Continental breakfast
8:30 – 10:15	PETSc Tutorial – Part 1 slides: 1 2 3 4 5
10:15 – 10:45	Break
10:45 – 12:30	PETSc Tutorial – Part 2
12:30 – 1:15	Working Lunch (start hands on)
1:15 – 2:15	Hands On / Interactive
2:15 – 2:45	Break (continue hands on)
2:45 – 3:15	TAO
3:15 – 3:45	SLEPc
3:45 – 4:30	MOOSE
4:30 – 5:00	Conclusion / Advanced Topics
5:00	Adjourn
5:00 – 6:00	Bus from Building 240 Conference Center to Argonne Guest House
6:30	Pre-conference Dinner @ Argonne Guest House

Celebrating 20 Years of Computational Science with PETSc
Conference Schedule

Tuesday, June 16

7:30 – 8:15 Bus from Argonne Guest to Building 240 Conference Center
8:00 – 8:30 Continental breakfast
8:30 – 10:00 (BS)[1]

8:30 Logistics, Welcome
Barry Smith, Argonne National Laboratory

9:00 *Optimization and Sensitivities of Time Dependent Simulations*
Hong Zhang, Argonne National Laboratory

9:30 *PCBDDC: Dual-Primal Preconditioners in PETSc*
Stefano Zampini, KAUST, Saudi Arabia

10:00 – 10:30 Break
10:30 –12:00 (BG)

10:30 *Simulations on Power Networks*
Shri Abhyankar, Argonne National Laboratory

11:00 *Distinct Solutions of Nonlinear PDEs via Deflation*
Patrick Farrell, Oxford University, England

11:30 *Schwarz for the "Outer-Loop"*
Xiao-Chuan Cai, University of Colorado, Boulder

12:00 – 1:00 Lunch/cafeteria
1:00 – 2:15 (LCM)

1:00 Panel 1: The Outer Loop

1:45 *Scalable Mesh and Data Management Using DMPlex*
Michael Lange, Imperial College, England and
Matthew Knepley, Rice University

2:15 – 2:45 Break
2:45 – 4:15 (MK)

2:45 *Three Dimensional Heating Rates in Cloud Resolving Models: Methods and Impact of Cloud Evolution and Precipitation*
Fabian Jakub, University of Munich, Germany

3:15 Lightning Talks 1
3:45 – 4:00 Break (set up posters)
4:00 – 5:30 Poster Session 1 (see list of posters on page 5)
5:30 Adjourn
5:30 – 6:15 Bus from Building 240 Conference Center to Argonne Guest House

6:30 Workshop Dinner @ Argonne Guest House

Panel 1: The Outer Loop: What needs to be done in algorithms, libraries, and applications to support computing sensitivities and optimizations of simulations as well as solving stochastic systems? Does this require refactoring/evolving the lower-level algorithm/software stack, i.e., PETSc? What level of abstraction should be used/exposed for the lower levels? For TS and SNES it is usually function evaluation plus Jacobian; should it be something else?
Moderator: Bill Gropp, University of Illinois at Urbana-Champaign
Panelists: Paul Bauman (SUNY Buffalo), Jed Brown (Argonne National Laboratory and University of Colorado, Boulder), Patrick Farrell (University of Oxford), Tobin Isaac (University of Texas at Austin)

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1 Moderator

Conference Schedule

Wednesday, June 17

7:30 – 8:15 Bus from Argonne Guest to Building 240 Conference Center
8:00 – 8:30 Continental breakfast
8:30 – 10:00 (HZ)

- 8:30 *SLEPc: Current Achievements and Plans for the Future*
  Jose Roman, Universitat Politècnica de València, Spain
- 9:00 *The Immersed Boundary Method for Advection-Electrodiffusion*
  Philhwa Lee, University of Michigan
- 9:30 *Gyrokinetic Particle-in-Cell Methods for Tokamak Edge Plasmas*
  Mark Adams, Lawrence Berkeley National Laboratory

10:00 – 10:30 Break
10:30 –12:30 (DK)

- 10:30 *PETSc: a SWOT Analysis,*
  David Keyes, KAUST, Saudi Arabia
- 11:00 *Fast Computation of Fully Resolved, Neuromechanically Driven Locomotion*,
  Namu Patel, Northwestern University
- 11:30 *15 years of PFLOTRAN,*
  Richard Mills, Intel
- 12:00 *PETSc on GPUs and MIC: Current Status and Future Directions*
  Karl Rupp, Vienna University of Technology, Austria

12:30 – 1:30 Lunch/cafeteria
1:30 – 3:45 (JB)

- 1:30 Panel 2: Leveraging the Community: Beyond Software Libraries
- 2:15 *Simplifying Multiphysics Through Application Composition*
  Derek Gaston, Idaho National Laboratory
- 2:45 *Scalable Parallel Solvers for Finite Elements and Isogeometric Discretizations in Computational Cardiology*
  Luca Pavarino, University of Milan, Italy

3:15 Lightning Talks 2
3:45 – 4:00 Break (set up posters)
4:00 – 5:00 Poster Session 2 (see list of posters on page 5)
5:00 – 6:00 Bus from Building 240 Conference Center to Argonne Guest House
5:00 Adjourn (Dinner on your own)

Panel 2: Leveraging the Community: Beyond Software Libraries: In mathematics, one builds new results using previously published theorems and proofs; publications, including books, are a fairly good vehicle to communicate results so that they may be reused. In numerical simulations, publications are unable to convey the depth of information required to leverage previous results. Application codes are rarely usable (or even buildable) beyond their original developers and thus are a poor way of leveraging previous work. Software libraries and packages have achieved success at enabling the leveraging of previous work. What other successful strategies exist for community leverage and reuse (e.g., StackExchange), and how can the impact of these approaches be measured fairly to prevent gaming the system?
Moderator: Matthew Knepley (Rice University)
Panelists: Derek Gaston (Idaho National Laboratory), Gerard Gorman (Imperial College), Glenn Hammond (Sandia National Laboratories), Jack Poulson (Stanford University)

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Conference Schedule

Thursday, June 18

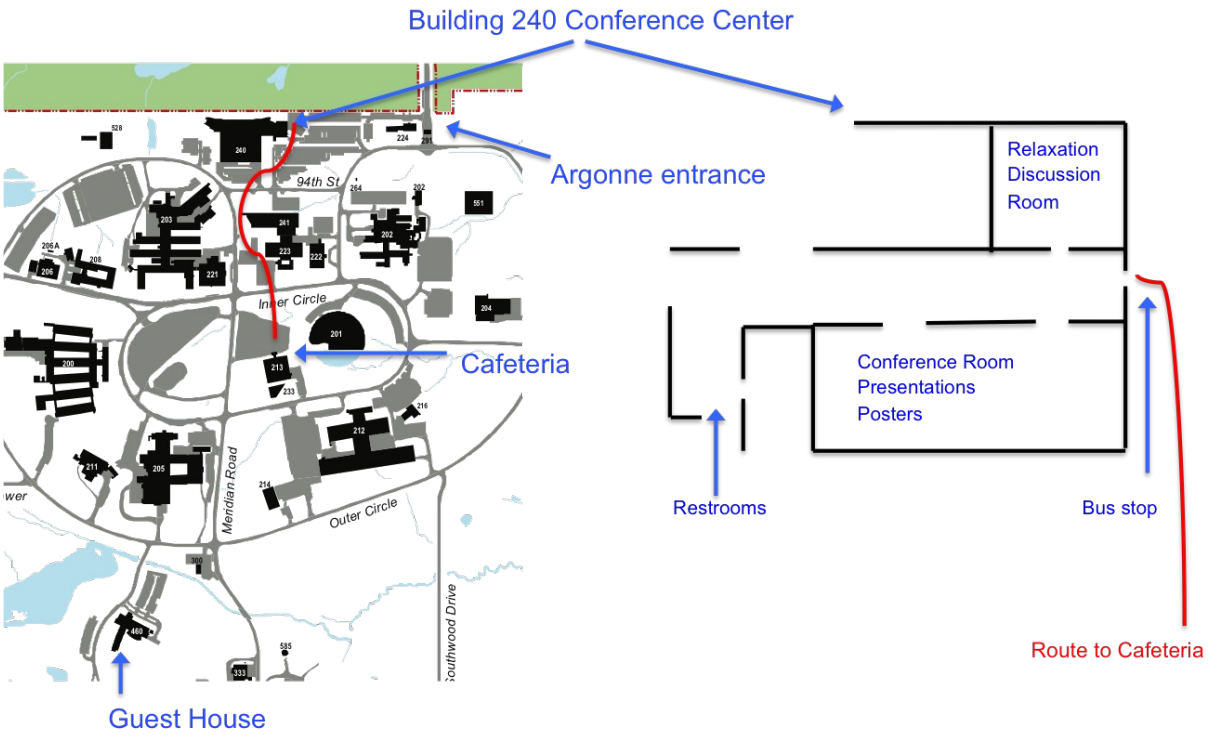
7:30 – 8:15 Bus from Argonne Guest to Building 240 Conference Center
8:00 – 8:30 Continental breakfast
8:30 – 10:00 (KR)

- 8:30 *PetIGA: A Framework for High Performance Isogeometric Analysis*, Lisandro Dalcin, KAUST, Saudi Arabia
- 9:00 *Current and Planned AMR support in PETSc* Tobin Isaac, University of Texas at Austin
- 9:30 *Solving the Load Flow and Helmholz Equations using PETSc* Domenico Lahaye, Delft University of Technology, Netherlands

10:00 – 10:30 Break
10:30 –12:00 (DK)

- 10:30 *PETSc in Computational Materials Science: Applications and Algorithmic Developments,* Dmitry Karpeyev, University of Chicago
- 11:00 *Computational Scale Bridging using PETSc on 458K Cores* Axel Klawonn, University of Cologne, Germany and Oliver Rheinbach, Technical University Bergakademie Freiberg, Germany
- 11:30 *How Not to Write Software Libraries* Bill Gropp, University of Illinois at Urbana-Champaign

12:00 Adjourn



Celebrating 20 Years of Computational Science with PETSc
Poster Presentations

Tuesday, June 16:

Multiscale Coevolution Algorithms for Nanosystems
Andrew Abi Mansour, Indiana University

Using PETSc to Develop an Unstructured Finite Element Code for Modeling Crustal Deformation
Sayed Tabrez Ali, University of Wisconsin, Madison

Enabling the "Outer Loop" with PETSc, libMesh, QUESO, and GRINS
Paul Bauman, SUNY Buffalo

Evaluating the Accuracy of Strategies for Generating Prediction Intervals for Natural Gas Demand Forecasts
William Castedo, Marquette University

Applying PETSc to a Three Dimensional Cloud Model Based on the Vector Vorticity Equation
Mu-Hua Chien, National Taiwan University

Anisotropic Mesh Optimisation via PETSc-DMPlex
Gerard Gorman, Imperial College, London

Firedrake: Automating Finite Element by Composing Abstractions
David Ham, Imperial College, London

Scalability of Shift-and-Invert Parallel Spectral Transformations for Quantum Chemistry Applications
Murat Keceli, Argonne National Laboratory

Wednesday, June 17:

High Fidelity Aerostructural Optimization
Gaetan Kenway, University of Michigan

Fully Resolved Simulation Model on Esophageal Transport
Wenjun (Walter) Kou, Northwestern University

PETSc-based Parallel Reduced-order Models for Earth Systems
Yaning Liu, Lawrence Berkeley National Laboratory

Building on PETSc's Multigrid Infrastructure in the Firedrake Finite Element Framework
Lawrence Mitchell, Imperial College, London

Pipelined, Flexible Krylov Methods
Patrick Sanan, Università della Svizzera Italiana

Parallelization of MIN3P-THCm: A High Performance Computational Framework for Subsurface Flow and Reactive Transport Simulation
Danyang Su, University of British Columbia

PETSc-based Parallel Semi-implicit CFD Code Gasflow-MPI in Application of Hydrogen Safety Analysis in Containment of Nuclear Power Plants
Jianjun Xiao, Karlsruhe Institute of Technology

SAWs: Scientific Application Web server
Hong Zhang, John O'Sullivan, Surtai Han, Matthew Otten, and the PETSc Team, Argonne National Laboratory